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Cumulative fatigue damage is known to be the leading cause of aircraft structural and engine failure. At the present time, reliable methods for prediction of fatigue crack initiation are not available, because the phenomenon starts at the atomic scale. Initiation of fatigue cracks is associated with the formation of persistent slip bands, which form inside metals with specific microstructure dimensions.

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ATOMISTIC-DISLOCATION DYNAMICS MODELLING OF FATIGUE MICROSTRUCTURE AND CRACK INITIATION

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Abstract

Cumulative fatigue damage is known to be the leading cause of aircraft structural and engine failure. At the present time, reliable methods for prediction of fatigue crack initiation are not available, because the phenomenon starts at the atomic scale. Initiation of fatigue cracks is associated with the formation of Persistent slip bands (PSBs), which form inside metals with specific microstructure dimensions. In this project, we developed computational methods that allow direct simulation of plasticity at the microstructure level, and can hence be used as a tool to study fatigue crack initiation. In one task of the project, a dislocation dynamics model that incorporates the influence of free and internal interfaces on dislocation motion was completed. The model is based on a self-consistent formulation of 3-D Parametric Dislocation Dynamics (PDD) with the Boundary Element method (BEM) to describe dislocation motion, and hence microscopic plastic flow in finite volumes. The developed computer models were bench-marked by detailed comparisons with the experimental data, developed at the Wright- Patterson Air Force Lab (WP-AFRL), by three dimensional large scale simulations of compression loading on micro-scale samples of FCC single crystals. In another task, we performed large-scale computer simulations of fatigue mechanisms in FCC metals and alloys to investigate the formation of ladder dislocation structures, the progressive development of PSBs, the interaction of irreversible slip events with external and internal surfaces, and the eventual nucleation of fatigue cracks in Ni-based superalloys. A summary of the project results is given here.

Research Objectives

The main objective of the research was to develop predictive and experimentally verified advanced computational capabilities for studying the plasticity of small volumes and the fatigue damage evolution. The methodology was based on fundamental material physics at the nano- and micro-scale, and was aimed at the development of microstructure-based models of fatigue damage in face center cubic metals and alloys. The overall objectives of the project can be summarized as follows:

1. Expand and upgrade the computational capabilities of the Parametric Dislocation Dynamics (PDD) at UCLA to include key new features, especially the effects of external/internal surface image forces by coupling the Boundary Element Method

(BEM) with the PDD method, and the interaction of dislocation ensembles with precipitates, the dislocation multiplication, and the dislocation annihilation processes.

2. The developed computer models are to be bench-marked with detailed comparisons with the experimental data base developed at the Wright- Patterson Air Force Lab (WP-AFRL) on micro-scale samples of FCC single crystals through. Large-scale 3-D computer simulations of micropillers under compression loading are to be performed, and from the simulation results an assessment of the crystal-size dependence of the stress versus strain response is to be analyzed for cylindrical FCC microcrystals. Statistical aspects of dislocation production from crystal surfaces, activation of internal dislocation sources, and the cross-slip process are included in this analysis.

3. The process of Persistent Slip Band (PSB) formation in FCC single crystals is to be investigated, and a clear quantitative understanding of the link between the evolution of PSBs and the fatigue limit in FCC metals is to be developed. These investigations are to be used to calibrate fatigue microstructure evolution physics that can lead to build fatigue damage practical and predictive models.

4. The process of crack nucleation will is to be investigated through detailed atomistic simulations.

In this report, we summarize some of the main results of the projects, and show that all project objectives have been met or exceeded.

Approach and Progress

Our approach here is to develop predictive computational capabilities for plasticity in finite volumes and fatigue damage evolution. Understanding dislocation interaction with free and internal surfaces (e.g. grain boundaries, precipitate surfaces, twin boundaries, voids, bubbles, and cracks) is essential in a wide range of applications, such as fatigue crack nucleation [1, 2], thin film deformation [3], and size effects on small sample plasticity [4, 5]. Discrete Dislocation Dynamics (DDD) has been developed to simulate plastic deformation at the meso-scale by direct numerical simulations of the collective motion of dislocation ensembles without ad hoc assumptions by direct numerical solution of the equations of motion. The approach has been successfully used in many applications at the nano- and micro-scales (e.g. [6-9]). However, the majority of these approaches are for bulk crystals, with a few exceptions that consider the influence of free or internal surfaces (e.g. [8, 10]). Careful assessments of the accuracy associated with these numerical methods would be helpful, especially because of the singular behavior of the elastic field of dislocations at free surfaces and interfaces.

An implementation of the Boundary Element Method (BEM) in dislocation dynamics simulations is developed to incorporate the influence of free and internal interfaces on dislocation motion. The computational structure of the PDD method has a great degree of similarity and consistency with the computations structure of the BEM. In the PDD, the fast sums are carried over quadrature points and the number of segments on each dislocation and the outer summation is over the number of dislocation loops, while the sums in the BEM are carried over the number of quadrature points twice and the number of nodes per element and the outer summation is finally performed over the number of surface elements. Thus, the computational

structure of both the PDD and the BEM is essentially the same. It is therefore convenient to model the effects of surface image forces with the BEM, while the computational structure of the PDD is unchanged. One possible additional advantage of this computational structure is the suitability of incorporating acceleration algorithms of conventional particle methods, and as the Greengard-Rokhlin fast multipole algorithms. By considering special cases for which analytical solutions are known, it is shown that the method is very accurate for calculating surface image forces on dislocations. By increasing the surface mesh density for BEM calculations, and the quadrature point density on dislocation segments, it is shown that the error can be controllably made to be small, and that the numerical solution displays absolute convergence.

The developed computer models are then bench-marked by detailed comparisons with the experimental data, developed at the Wright- Patterson Air Force Lab (WP-AFRL), by three dimensional large scale simulations of compression loading on micro-scale samples of FCC single crystals. The plastic flow characteristics as well as the stress-strain behavior of simulated micropillars are shown to be in general agreement with experimental observations.

The singular nature of the stress field of dislocations limits the resolution capability of DD simulations to 2-3 lattice constants from internal or external surfaces. Additionally, stress-induced phase transformations, shearing, cross-slip, looping around precipitates cannot be predicted by dislocation theory. The formation conditions of surface cracks are also atomic in nature and this type of information must be supplied to DD simulations for accurate predictions of dislocation interactions outcomes.

MD Simulations of Dislocation Nucleation

The limitations of our proposed PDD-BEM method was addressed by informing these simulations from the results of atomistic Molecular Dynamics (MD) calculations. These limitations are: (1) nucleation conditions and rates of dislocation loops, (2) singularity of the stress field at interfaces, precipitates and boundaries, and (3) re-configuration of precipitates or other small obstacles to dislocation motion by shearing or total destruction. We designed simulations on single dislocations using the MD technique, and then passed this information to larger systems for more detailed DD simulations. The MD simulations were performed on copper and nickel to study the interaction of dislocations with (a) external surfaces, (b) grain boundary, and (c) γ'-precipitates. Mishin potentials, which have been calibrated, to reproduce ab initio values of stacking fault energies were used in these

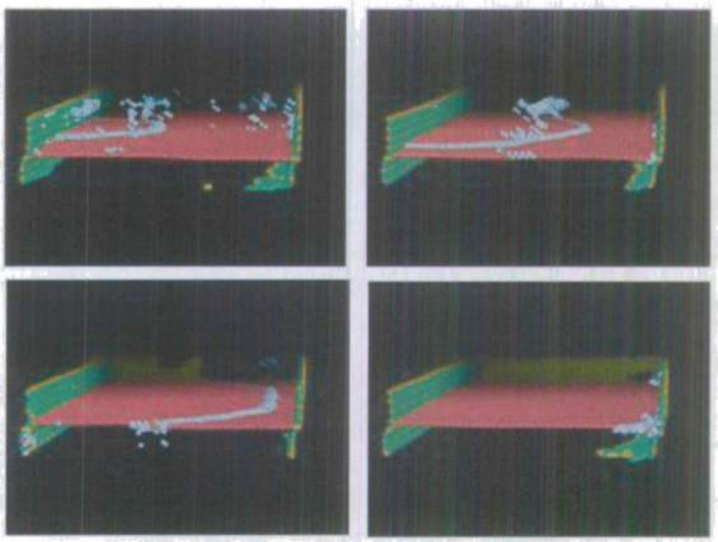

Fig 1. Atomistic Simulations of twin-boundary dislocation nucleation from a free surface

calculations. Defects inside the simulation cell are visualized by a local crystallinity classification method that, to capture both the number of nearest neighbors and the central symmetry character of individual atoms. In addition, we have implemented the atomistic Nye tensor analysis developed by Hartley and Mishin [12] to identify the dislocation character of defected zones. Stress-strain relations are also calculated. From these result it is possible to determine the nature of the deformation mechanism and the outcomes of dislocation interaction with various boundaries. An example of the mechanism of dislocation loop nucleation from a twin boundary is shown in Fig. 1.

Dislocation Dynamics Simulations of Micro-Plasticity

As an application of the current methodology, the PDD-BEM was utilized to study the size effects and the single-slip behavior of micropillars through a large scale 3-dimensional simulation that mimics the experimental conditions [4, 5]. The plastic response of micropillars under compression loading for sizes in the range of $D = 0.25 - 5.0$ μm is studied. The size effects on the flow stress are clearly observed and the results are in complete agreement with experimental observations. Plastic flow arises from the collective motion of dislocations within the volume of the micropillars. The effect of applying a strain controlled loading versus a stress controlled loading is studied and shown in Fig. 2-(a) for different micropillar sizes. In addition, a number of parameters and mechanisms (e.g. micropillar size, average length of activated single-pinned dislocations, and cross-slip activation) are examined in an effort to identify size scaling aspects of plastic flow and work-hardening. It is observed that plastic flow is intermittent and not continuous. By a thorough study of the microstructure evolution, the observed size effects on the flow strength are rationalized here on the basis of a statistical variation in the length of single-pinned dislocation sources in the crystal. In addition, a number of scaling laws that relate the flow strength to the micropillar diameter, and the average length of activated single-pinned

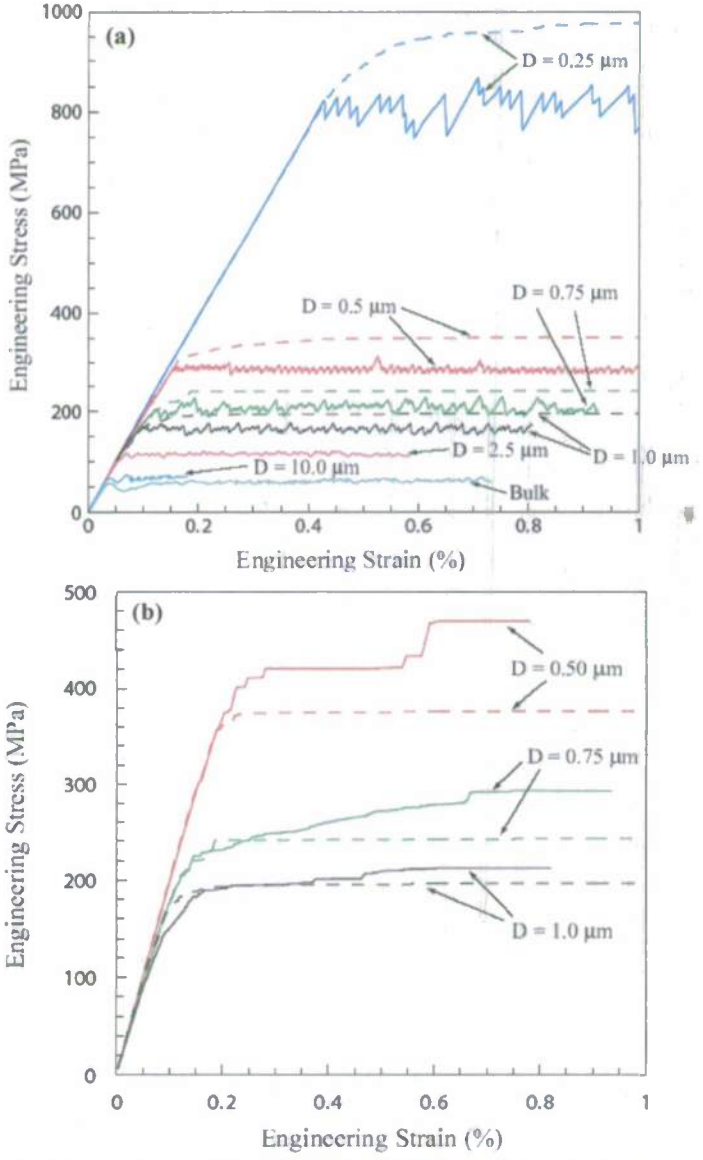

Fig. 2. Stress-strain relations for: (a) simulations without cross-slip activation using a strain controlled technique (solid lines) and stress controlled technique (dashed lines); (b) simulations using stressed controlled technique with cross-slip activation (solid lines) and without cross-slip activation (dashed lines).

dislocations were developed. The dislocation density evolution is observed to be cyclic and a Fast Fourier Transform analysis revealed that dislocation activities in the volume are cyclical as well. In addition, the activation of cross-slip is shown to have a significant effect on work-hardening (Fig. 2-(b)). Finally, the observed size effects are shown to be consistent with a "weakest-link activation mechanism".

Simulations of Saturated Fatigue Strength

In addition, we devloped models of localized plastic deformation inside Persistent Slip Band channels. The interaction between screw dislocations as they pass one another inside channel walls in copper was investigated. The model showed the mechanisms of dislocation bowing, dipole formation and binding, and finally dipole destruction as screw dislocations pass one another. The mechanism of (dipole passing) was assessed and interpreted in terms of the fatigue saturation stress. We also presented results for the effects of the wall dipole structure on the dipole passing mechanism. Details of the shape of the screw dislocations as they simultaneously bow out in between the walls are seen to have a considerable effect on the passing stress, thus validating the need for accurate DDD simulations. In Fig. 3, the passing stress (Maximum applied resolved shear stress) as a function of the initial distance between the screw dislocations. Different analytical estimates are shown in addition to the dislocation dynamics results. In addition, the long range internal stress field in the edge dislocation dipolar walls is seen to have an effect on the passing stress as well. It follows that the passing stress in the middle of the channel is reduced to the following limits: $16.8 \leq \tau_{pass} \leq 20$ MPa, which is in agreement with the well-established fact that the stress acting locally in the channels of the heterogeneous PSB structure are modified markedly from the macroscopically applied value by long-range internal stresses [13]. In fact, it is reported that the stress acting locally in the channel is lowered to about 16 to 17 MPa [13], which is in reasonable agreement with the current numerical predictions. Finally, from large scale simulations of the expansion process of the edge dipoles from the walls in the channel

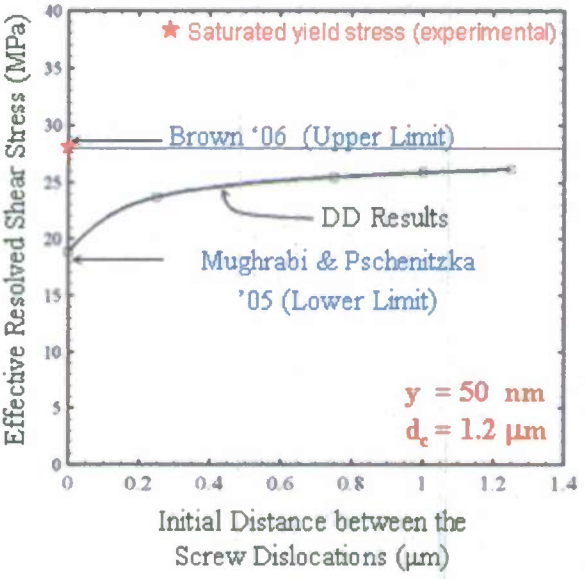

Fig. 3. Passing stress (Maximum applied resolved shear stress) as a function of the initial distance between the screw dislocations

Simulations of Fatigue Hysteresis Loops & PSB Microstructure

We performed large-scale simulations of the expansion process of the edge dipoles from the walls in of PSB channels. This gave a better assessment of the stress distribution throughout the channel and the effect of the long range internal stress field. An interesting outcome from these simulations is that screw dislocations in the PSB channels may not meet "symmetrically", i.e. precisely in the center of the channel but preferably a little on one or the other side. For this

configuration the passing stress will be lowered which is in agreement to experimental observations [14]. Representative results of these simulations are shown in the Figures (4-6) below.

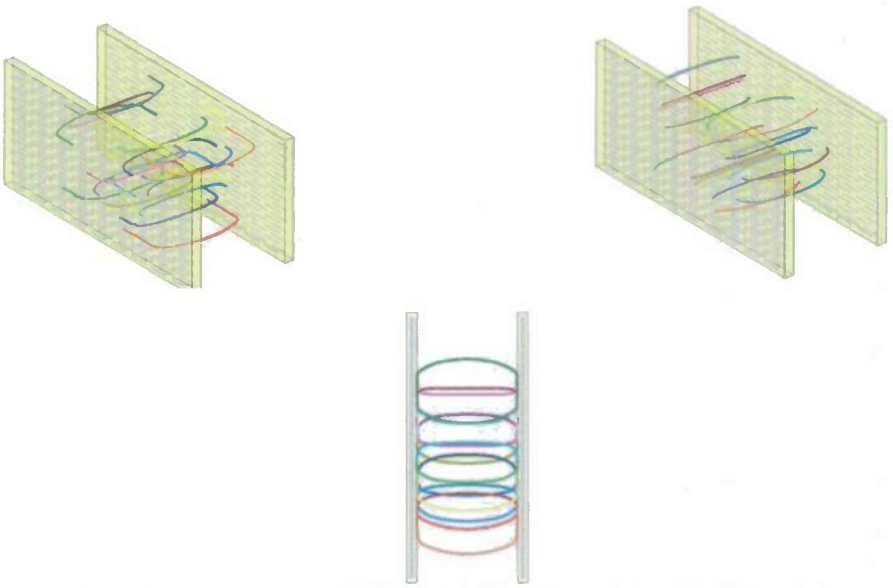

Figure 4: Dislocation Microstructure within the PSB channel (3D - top), and plan view (bottom)

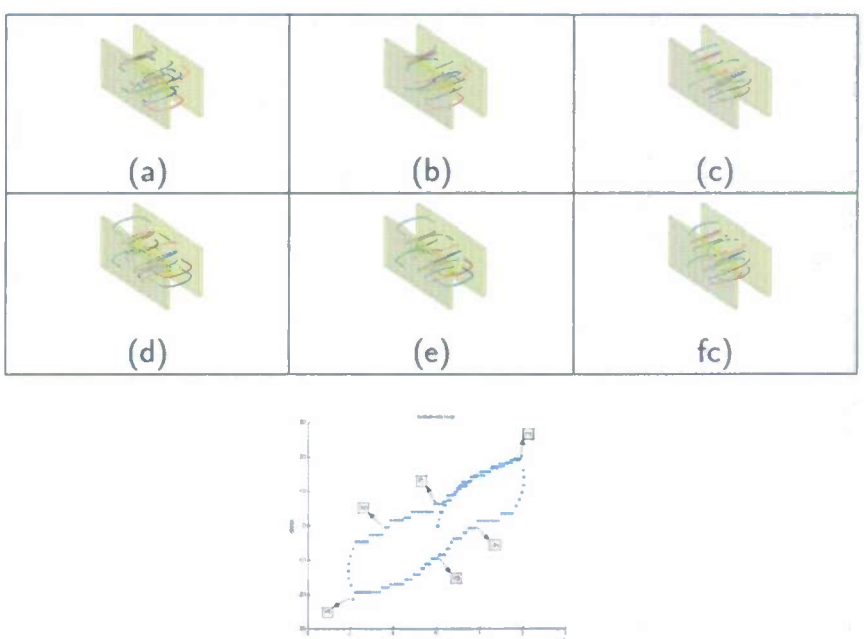

Figure 5: Successive PSB dislocation microstructure corresponding to a full fatigue hysteresis loop (bottom)

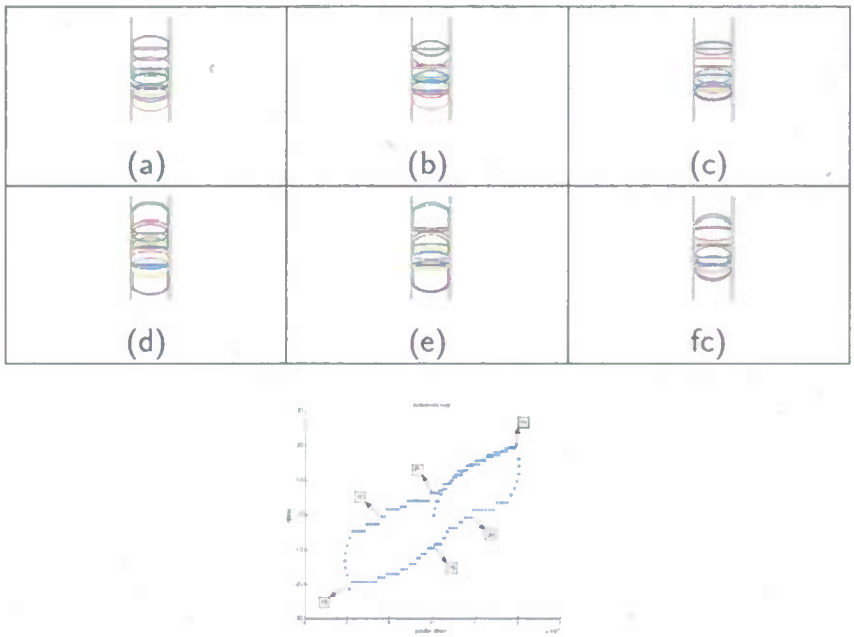

Figure 6: Plan view of fatigue dislocation microstructure and corresponding stress-strain hysteresis loop.

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Can Erel	Current Ph.D. student at UCLA. Can will finish his Ph.D. thesis by next year.
Nasr Ghoniem	Professor, University of California, Los Angeles

Publications

(1) J.A. El-Awady, M. Wen and N.M. Ghoniem, "The Role of the Weakest Link Mechanism in Controlling the Plasticity of Micropillars", Journal of the Mechanics and Physics of Solids, **57(1)**, 32-50, 2009.

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Awards Received

Jaafar El-Awady	Outstanding Ph.D. in Aerospace Engineering, University of California, Los Angeles
Nasr M. Ghoniem	Awarded Fellow of the American Academy of Mechanics.

Transitions

None during this period.